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# Towards improved photovoltaic conversion using dilute magnetic semiconductors

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## Abstract

Present photovoltaic devices, based on p/n junctions, are limited from first principles to maximal efficiencies of 31% (40% under full solar concentration; Shockley and Queisser 1961 *J. Appl. Phys.* **32** 510). However, more innovative schemes may overcome the Shockley–Queisser limit since the theoretical maximal efficiency of solar energy conversion is higher than 85% (Harder and Würfel 2003 *Semicond. Sci. Technol.* **18** S151). To date, the only practical realization of such an innovative scheme has been multi-junction devices, which at present hold the world record for efficiency at nearly 41% at significant solar concentration (US DOE news site: <http://www.energy.gov/news/4503.htm>). It has been proposed that one could make use of the solar spectrum in much the same way as the multi-junction devices do but in a single cell, using impurity induced intermediate levels to create gaps of different sizes. This intermediate level semiconductor (ILSC) concept (Green and Wenham 1994 *Appl. Phys. Lett.* **65** 2907; Luque and Martí 1997 *Phys. Rev. Lett.* **78** 5014) has a maximal efficiency similar to that of multi-junction devices but suffers from prohibitively large non-radiative recombination rates.

We here propose to use a ferromagnetic impurity scheme in order to reduce the non-radiative recombination rates while maintaining the high theoretical maximum efficiency of the ILSC scheme, that is about 46%. Using density functional theory calculations, the electronic and energetic properties of transition metal impurities for a wide range of semiconductors have been analysed. Of the several hundred compounds studied, only a few fulfil the design criteria that we present here. As an example, wide gap AIP is one of the most promising compounds. It was found that inclusion of significant amounts of Mn in AIP induces band structures providing conversion efficiencies potentially close to the theoretical maximum, with an estimated Curie temperature reaching above 100 K.